2-(6,7,8,9-tetrahydro-5H-carbazol-3-yl)acetonitrile
57411-92-4 | DTXSID10306303

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	1.14	0.85	1.12	0.83	1.23

Model Results

Predicted value: 2.02e-10 cm3/molecule*sec

Global applicability domain: Outside

Local applicability domain index: 1.89e-01

Confidence level: 8.25e-01

Nearest Neighbors from the Training Set

Image not found
alpha-Humalene
Measured: 2.90e-10
Predicted: 2.87e-10

Image not found
alpha-Phellandrene
Measured: 3.13e-10
Predicted: 2.83e-10

Image not found
alpha-Terpinene
Measured: 3.63e-10
Predicted: 2.91e-10

Image not found
gamma-Terpinene
Measured: 1.77e-10
Predicted: 2.06e-10

Image not found
Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
Measured: 4.80e-11
Predicted: 4.73e-11